Nonadiabatic Geometric Phase
in Quaternionic Hilbert Space

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ABSTRACT

We develop the theory of the nonadiabatic geometric phase, in both
the Abelian and non-Abelian cases, in quaternionic Hilbert space.

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1. Introduction

The theory of geometric phases associated with cyclic evolutions of a physical system is now a well-developed subject in complex Hilbert space. The seminal work of Berry on the adiabatic single state (Abelian) case [1] has been extended to the non-Abelian case of the adiabatic evolution of a set of degenerate states [2], and both of these have been further extended [3, 4] to show that there is a geometric phase associated with any cyclic but nonadiabatic evolution of a single quantum state or of a degenerate group of quantum states.

In this paper we take up another direction for generalization of the geometric phase, from quantum mechanics in complex Hilbert space to quantum mechanics [5, 6] in quaternionic Hilbert space. The generalization of the adiabatic geometric phase to quaternionic Hilbert space was given in Ref. 6, where it was shown that for states of nonzero energy the adiabatic geometric phase is complex, as opposed to quaternionic, with a quaternionic adiabatic geometric phase occurring only for the adiabatic cyclic evolution of zero energy states. Consideration of nonadiabatic cyclic evolutions was also begun in Ref. 6, but the discussion given there is incomplete. While Sec. 5.8 of Ref. 6 constructed a nonadiabatic cyclic invariant phase, it did not address the problem of separating this phase into a dynamical part determined by the quantum mechanical Hamiltonian, and a geometric part that depends only on the ray orbit and is independent of the Hamiltonian.

The purpose of the present paper is to give a complete discussion of the nonadiabatic geometric phase in quaternionic Hilbert space. In Sec. 2 we give a very brief survey of the properties of quantum mechanics in quaternionic Hilbert space that are needed in the analysis that follows. In Sec. 3 we consider the cyclic nonadiabatic evolution of a single quantum

state, and show how to explictly generalize to quaternionic Hilbert space the construction of a nonadiabatic geometric phase given in Ref. 3. In Sec. 4 we extend our analysis to the case of a degenerate group of states, thereby obtaining a quaternionic nonadiabatic non-Abelian geometric phase corresponding to the complex construction given in Ref. 4. A brief summary and discussion of our results is given in Sec. 5.

2. Quantum Mechanics in Quaternionic Hilbert Space

Only a few properties of quaternionic quantum mechanics are needed for the discussion that follows; the reader wishing to learn more than we can present here should consult Ref. 6. In quaternionic quantum mechanics, the Dirac transition amplitudes $\langle \psi | \phi \rangle$ are quaternion valued, that is, they have the form

$$\langle \psi | \phi \rangle = r_0 + r_1 i + r_2 j + r_3 k \; , \tag{1}$$

where $r_{0,1,2,3}$ are real numbers and where i, j, k are quaternion imaginary units obeying the associative algebra $i^2 = j^2 = k^2 = -1$ and $ij = -ji = k$, $jk = -kj = i$, $ki = -ik = j$. Because quaternion multiplication is noncommutative, two independent Dirac transition amplitudes $\langle \psi | \phi \rangle$ and $\langle \kappa | \eta \rangle$ in general do not commute with one another, unlike the situatation in standard complex quantum mechanics, where all Dirac transition amplitudes are complex numbers and mutually commute. The transition probability corresponding to the amplitude of Eq. (1) is given by

$$P(\psi, \phi) = |\langle \psi | \phi \rangle|^2 \equiv \overline{\langle \psi | \phi \rangle} \langle \psi | \phi \rangle = r_0^2 + r_1^2 + r_2^2 + r_3^2 \; , \tag{2}$$

where the bar denotes the quaternion conjugation operation $\{i, j, k\} \to \{-i, -j, -k\}$ and where we have assumed the states $|\psi\rangle$ and $|\phi\rangle$ to be unit normalized. Since the quaternion

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norm defined by Eq. (2) has the multiplicative norm property

$$|q_1 q_2| = |q_1| \, |q_2| \, ,$$ (3)

the transition probability of Eq. (2) is unchanged when the state vector $|\phi\rangle$ is right multiplied by a quaternion ω of unit magnitude,

$$|\phi\rangle \rightarrow |\phi\rangle\omega, \quad |\omega| = 1 \quad \Rightarrow P(\psi, \phi) \rightarrow P(\psi, \phi) \, .$$ (4)

Hence as in complex quantum mechanics, physical states are associated with Hilbert space rays of the form $\{|\phi\rangle\omega \, : \, |\omega| = 1\}$, and the transition probability of Eq. (2) is the same for any ray representative state vectors $|\psi\rangle$ and $|\phi\rangle$ chosen from their corresponding rays. In the next section, we shall follow Ref. 3 in denoting quaternionic Hilbert space by $\mathcal{H}$, and the projective Hilbert space of rays of $\mathcal{H}$ by $\mathcal{P}$.

Time evolution of the state vector $|\psi\rangle$ is described in quaternionic quantum mechanics by the Schrödinger equation

$$\frac{\partial|\psi\rangle}{\partial t} = -\tilde{H}|\psi\rangle \, ,$$ (5a)

with

$$\tilde{H} = -\tilde{H}^\dagger$$ (5b)

an anti-self-adjoint Hamiltonian. From Eqs. (5a, b) we see that the Dirac transition amplitude $\langle\psi|\phi\rangle$ is time independent,

$$\frac{\partial}{\partial t}\langle\psi|\phi\rangle = (\frac{\partial}{\partial t}\langle\psi|)|\phi\rangle + \langle\psi|\frac{\partial}{\partial t}|\phi\rangle$$
$$= \langle\psi|\tilde{H} - \tilde{H}|\phi\rangle = 0 \, ,$$ (6)

and thus the Schrödinger dynamics of state vectors preserves the inner product structure of Hilbert space. The dynamics of Eqs. (5, 6) is evidently preserved under right linear

superposition of states with quaternionic constants,

$$\frac{\partial|\psi\rangle}{\partial t} = -\tilde{H}|\psi\rangle \ , \frac{\partial|\phi\rangle}{\partial t} = -\tilde{H}|\phi\rangle \quad \Rightarrow$$

$$\frac{\partial(|\psi\rangle q_1 + |\phi\rangle q_2)}{\partial t} = -\tilde{H}(|\psi\rangle q_1 + |\phi\rangle q_2) \ . \tag{7}$$

Equation (7) illustrates two general features of our conventions for quaternionic quantum mechanics, which are that linear operators (such as $\tilde{H}$) act on Hilbert space state vectors by multiplication from the left, whereas quaternionic numbers (the scalars of Hilbert space) act on state vectors by multiplication from the right. Adherence to these ordering conventions is essential because of the noncommutative nature of quaternionic multiplication.

3. The Nonadiabatic Abelian Quaternionic Geometric Phase

Let us now consider a unit normalized quaternionic Hilbert space state $|\psi(t)\rangle$ which undergoes a cyclic evolution between the times $t = 0$ and $t = T$. Since physical states are associated with rays, this means that

$$|\psi(T)\rangle = |\psi(0)\rangle\Omega \ , \quad |\Omega| = 1 \ , \tag{8}$$

and so the orbit $\mathcal{C}$ of $|\psi(t)\rangle$ in $\mathcal{H}$ projects to a closed curve $\hat{\mathcal{C}}$ in the projective Hilbert space $\mathcal{P}$.

Let us now define a state $|\hat{\psi}(t)\rangle$ that is equal to $|\psi(t)\rangle$ at $t = 0$, that differs from $|\psi(t)\rangle$ only by a reraying at general times, i.e.,

$$|\psi(t)\rangle = |\hat{\psi}(t)\rangle\hat{\omega}(t) \ ,$$

$$|\hat{\omega}(t)| = 1 \ , \tag{9a}$$

$$\hat{\omega}(0) = 1 \ ,$$

and that evolves in time by parallel transport, i.e.,

$$\langle\hat{\psi}(t)|\frac{\partial|\hat{\psi}(t)\rangle}{\partial t} = 0 \ . \tag{9b}$$

The conditions of Eqs. (9a, b) uniquely determine $\hat{\omega}(t)$, and hence the state $|\hat{\psi}(t)\rangle$, as follows. Substituting the first line of Eq. (9a) into the Schrödinger equation of Eq. (5a), we get

$$
\begin{aligned}
-\tilde{H}|\hat{\psi}(t)\rangle\hat{\omega}(t) = & -\tilde{H}|\psi(t)\rangle \\
= & \frac{\partial|\psi(t)\rangle}{\partial t} = |\hat{\psi}(t)\rangle\frac{d\hat{\omega}(t)}{dt} + \frac{\partial|\hat{\psi}(t)\rangle}{\partial t}\hat{\omega}(t) \ .
\end{aligned}
\tag{10}
$$

Taking the inner product of this equation with the state $\langle\hat{\psi}(t)|$, and using the unit normalization of the state vector $|\hat{\psi}(t)\rangle$ together with the parallel transport condition of Eq. (9b), we get

$$
\frac{d\hat{\omega}(t)}{dt} = -\langle\hat{\psi}(t)|\tilde{H}|\hat{\psi}(t)\rangle\hat{\omega}(t) \ .
\tag{11}
$$

This differential equation can be immediately integrated to give

$$
\hat{\omega}(t) = T_\ell e^{-\int_0^t dv\langle\hat{\psi}(v)|\tilde{H}|\hat{\psi}(v)\rangle} \ ,
\tag{12}
$$

where T_ℓ denotes the time ordered product which orders later times to the left, and where we have used the initial condition on the third line of Eq. (9a). In particular, Eq. (12) gives us a formula for the value $\hat{\omega}(T)$ at the end of the cyclic evolution. We shall see that this has the interpretation of the dynamics-dependent part of the total phase change Ω.

To relate Eq. (12) to the total phase change, we use Eqs. (8) and (9a) to write

$$
|\hat{\psi}(T)\rangle\hat{\omega}(T) = |\psi(T)\rangle = |\psi(0)\rangle\Omega = |\hat{\psi}(0)\rangle\Omega \ ,
\tag{13a}
$$

so that taking the inner product with $\langle\hat{\psi}(0)|$ gives

$$
\Omega = \langle\hat{\psi}(0)|\hat{\psi}(T)\rangle\hat{\omega}(T) \ .
\tag{13b}
$$

To complete the calculation, we must now evaluate the inner product appearing in Eq. (13b). To do this, we introduce a third state vector $|\tilde{\psi}(t)\rangle$ which differs from $|\hat{\psi}(t)\rangle$ by a change of

ray representative, by writing

$$|\hat{\psi}(t)\rangle = |\tilde{\psi}(t)\rangle \tilde{\omega}(t) ,$$

$$|\tilde{\omega}(t)| = 1 , \tag{14a}$$

$$\tilde{\omega}(0) = 1 ,$$

and by requiring that $\tilde{\psi}$ should be continuous over the orbit $\mathcal{C}$,

$$|\tilde{\psi}(T)\rangle = |\tilde{\psi}(0)\rangle . \tag{14b}$$

Differentiating the first line of Eq. (14a) with respect to time, we get

$$\frac{\partial |\hat{\psi}(t)\rangle}{\partial t} = \frac{\partial |\tilde{\psi}(t)\rangle}{\partial t} \tilde{\omega}(t) + |\tilde{\psi}(t)\rangle \frac{d\tilde{\omega}(t)}{dt} . \tag{15}$$

Taking the inner product of Eq. (15) with $\tilde{\omega}(t)\langle\hat{\psi}(t)|$, using the parallel transport condition of Eq. (9b) together with the first line of Eq. (14a), and abbreviating the time derivative $\frac{\partial}{\partial t}$ by a dot, we obtain

$$0 = \langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle \tilde{\omega}(t) + \langle\tilde{\psi}(t)|\tilde{\psi}(t)\rangle \dot{\tilde{\omega}}(t) . \tag{16a}$$

Since the second line of Eq. (14a) implies that the state $|\tilde{\psi}(t)\rangle$ is unit normalized, Eq. (16a) simplifies to

$$\dot{\tilde{\omega}}(t) = -\langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle \tilde{\omega}(t) , \tag{16b}$$

which can be immediately integrated to give

$$\tilde{\omega}(t) = T_\ell e^{-\int_0^t dv \langle\tilde{\psi}(v)|\dot{\tilde{\psi}}(v)\rangle} , \tag{17}$$

with T_ℓ as before indicating a time ordered product. In particular, Eq. (17) gives us a formula for $\tilde{\omega}(T)$. But from Eqs. (14a, b) we have

$$|\hat{\psi}(T)\rangle = |\tilde{\psi}(T)\rangle \tilde{\omega}(T) = |\tilde{\psi}(0)\rangle \tilde{\omega}(T) = |\hat{\psi}(0)\rangle \tilde{\omega}(T) , \tag{18a}$$

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and so taking the inner product of Eq. (18a) with $\langle \hat{\psi}(0)|$ we get

$$\langle \hat{\psi}(0)|\hat{\psi}(T)\rangle = \tilde{\omega}(T) \ , \tag{18b}$$

determining the inner product appearing in Eq. (13b).

We thus get as our final result,

$$\Omega = \Omega_{\text{geometric}} \Omega_{\text{dynamical}} \ , \tag{19a}$$

with

$$\Omega_{\text{geometric}} \equiv \tilde{\omega}(T) = T_\ell e^{-\int_0^T dv \langle \tilde{\psi}(v)|\dot{\tilde{\psi}}(v)\rangle} \ , \tag{19b}$$

and with

$$\Omega_{\text{dynamical}} \equiv \hat{\omega}(T) = T_\ell e^{-\int_0^T dv \langle \hat{\psi}(v)|\tilde{H}|\hat{\psi}(v)\rangle} \ . \tag{19c}$$

The dynamical part of the phase is so called because it depends explicitly on $\tilde{H}$, as well as

on the orbit $\hat{\mathcal{C}}$ in the projective Hilbert space $\mathcal{P}$; it is uniquely determined by the conditions

of Eqs. (9a, b), since these conditions uniquely determine the state $|\hat{\psi}(t)\rangle$. The geometric

part of the phase is so called because, as we shall now show, it depends uniquely on the

projective orbit $\hat{\mathcal{C}}$ up to an overall quaternion automorphism transformation. To see this,

let us make the reraying

$$|\tilde{\psi}(t)\rangle \rightarrow |\tilde{\psi}'\rangle\omega'(t), \quad |\omega'| = 1 \ , \tag{20a}$$

with $\omega'(t)$ continuous over the orbit $\mathcal{C}$ so that

$$\omega'(T) = \omega'(0) \ . \tag{20b}$$

Then (as shown in detail in Sec. 5.8 of Ref. 6) the properties of the time ordered integral in

Eq. (19b) imply that under this transformation,

$$\Omega_{\text{geometric}} \rightarrow \overline{\omega}'(T)\Omega_{\text{geometric}} \omega'(0) \ , \tag{21a}$$

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which by the continuity condition of Eq. (20b) reduces to the quaternion automorphism transformation

$$\Omega_{\text{geometric}} \to \overline{\omega}'(0)\Omega_{\text{geometric}}\,\omega'(0) \ . \tag{21b}$$

Since for any two quaternions q_1, q_2 we have $\operatorname{Re} q_1 q_2 = \operatorname{Re} q_2 q_1$, with Re denoting the real part, Eq. (21b) implies that

$$\cos \gamma_{\text{geometric}} \equiv \operatorname{Re}\Omega_{\text{geometric}} \tag{22}$$

is a reraying invariant, and thus $\gamma_{\text{geometric}}$ is a nonadiabatic geometric phase angle that is a property solely of the projective orbit $\hat{\mathcal{C}}$. The fact that the nonadiabatic geometric phase in quaternionic Hilbert space is only determined modulo π is a reflection of the fact that $e^{i\gamma}$ is changed to $e^{-i\gamma}$ by the quaternion automorphism transformation

$$e^{-i\gamma} = \bar{j}e^{i\gamma}j \ . \tag{23}$$

Thus, to recover the result that the complex nonadiabatic geometric phase is determined modulo 2π by embedding a complex Hilbert space in a quaternionic one and using Eqs. (19a-c), one must exclude the possibility of making intrinsically quaternionic automorphism transformations involving the quaternion units j or k, as in Eq. (23).

In geometric terms, $\Omega_{\text{geometric}}$ is the holonomy transformation of the connection $A \equiv \langle \tilde{\psi} | d\tilde{\psi} \rangle$. But since this connection is quaternion-imaginary valued, it is analogous to an $SO(3)$ gauge potential. Therefore, the corresponding curvature is of the Yang-Mills type and is given by $F = dA + A \wedge A$.

An alternative expression for the total phase change Ω can be obtained [7] by writing

$$|\psi(t)\rangle = |\tilde{\psi}(t)\rangle \tilde{\chi}(t) \ ,$$

$$\tilde{\chi}(t) = \hat{\omega}(t)\tilde{\omega}(t) \ , \quad \tilde{\chi}(0) = 1 \ . \tag{24}$$

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Substituting Eq. (24) into the Schrödinger equation and then taking the inner product with $\langle\tilde{\psi}(t)|$, we obtain

$$\frac{d\tilde{\chi}(t)}{dt} = -(\langle\tilde{\psi}(t)|\tilde{H}|\tilde{\psi}(t)\rangle + \langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle)\tilde{\chi}(t) \ , \tag{25a}$$

which can be integrated from 0 to T to give

$$\Omega = T_\ell e^{-\int_0^T dv(\langle\tilde{\psi}(v)|\tilde{H}|\tilde{\psi}(v)\rangle + \langle\tilde{\psi}(v)|\dot{\tilde{\psi}}(v)\rangle)} \ . \tag{25b}$$

This procedure and the resulting formula of Eq. (25b) are direct analogs of the derivation given in Ref. 3 for the complex Hilbert space case, but in quaternionic Hilbert space the two terms in the exponential are noncommutative, and so the exponential in Eq. (25b) cannot be immediately factored into dynamical and geometric phase factors. As we have seen, to achieve this factorization it is necessary to use a two-step procedure, involving the parallel transported state $|\hat{\psi}(t)\rangle$ as well as the state $|\tilde{\psi}(t)\rangle$ that is continuous over the cycle.

4. The Nonadiabatic Non-Abelian Quaternionic Geometric Phase

We turn next to the quaternionic Hilbert space generalization of the complex nonadiabatic [4] non-Abelian [2] geometric phase. We consider now a cyclic evolution in a n-dimensional Hilbert subspace V_n, i.e., $V_n(T) = V_n(0)$. Let $|\psi_a(t)\rangle$, $a = 1, ..., n$ be a complete orthonormal basis for V_n, so that the reraying invariant projection operator for V_n is

$$\rho_n(t) = \sum_{a=1}^n |\psi_a(t)\rangle\langle\psi_a(t)| \ , \tag{26a}$$

in terms of which the cyclic evolution condition takes the form

$$\rho_n(T) = \rho_n(0) \ . \tag{26b}$$

Expressed in terms of the state vectors of the basis, the invariance of V_n implies that the basis element $|\psi_b(T)\rangle$ must be a superposition of the basis elements $|\psi_a(0)\rangle$, multiplied from the right by quaternionic coefficients U_{ab},

$$|\psi_b(T)\rangle = \sum_{a=1}^{n} |\psi_a(0)\rangle U_{ab} \ . \tag{27}$$

Substituting Eq. (27) into Eqs. (26a, b), we find that invariance of the projection operator requires

$$\begin{aligned}
\rho_n(T) &= \sum_{b=1}^{n} |\psi_b(T)\rangle\langle\psi_b(T)| \\
&= \sum_{a,b,c=1}^{n} |\psi_a(0)\rangle U_{ab}\overline{U}_{cb}\langle\psi_c(0)| \\
&= \sum_{a=1}^{n} |\psi_a(0)\rangle\langle\psi_a(0)| = \rho_n(0) \ ,
\end{aligned} \tag{28a}$$

which implies that

$$\sum_{b=1}^{n} U_{ab}\overline{U}_{cb} = \delta_{ac} \ . \tag{28b}$$

Similarly, orthonormality of the basis at $t = 0$ and $t = T$ implies that

$$\begin{aligned}
\delta_{ab} &= \langle\psi_a(T)|\psi_b(T)\rangle = \sum_{c,d=1}^{n} \overline{U}_{ca}\langle\psi_c(0)|\psi_d(0)\rangle U_{db} \\
&= \sum_{c,d=1}^{n} \overline{U}_{ca}\delta_{cd} U_{db} = \sum_{d=1}^{n} \overline{U}_{da} U_{db} \ .
\end{aligned} \tag{28c}$$

Hence U is a $n \times n$ quaternion unitary matrix, $U^\dagger U = UU^\dagger = 1$, that replaces the quaternion phase Ω (which is a 1×1 quaternion unitary matrix) of the preceding section.

Thus, to generalize the results of the preceding section to the non-Abelian case (i) one replaces the state vectors $|\psi\rangle, |\hat{\psi}\rangle, |\tilde{\psi}\rangle$ by n-component column vectors $|\psi_a\rangle, |\hat{\psi}_a\rangle, |\tilde{\psi}_a\rangle$, $a = 1, ..., n$, (ii) one replaces the phases $\Omega, \hat{\omega}, ...$ by $n \times n$ quaternion unitary matrices acting on

the state vector indices, (iii) one replaces Re in Eq. (22) by ReTr, with Tr the trace over the subspace V_n, and (iv) as in Ref. 4, one generalizes the parallel transport condition

of Eq. (9b) to

$$\langle \hat{\psi}_a(t) | \frac{\partial |\hat{\psi}_b(t)\rangle}{\partial t} = 0 \ , \quad a, b = 1, ..., n. \tag{28d}$$

The principal difference from the complex case treated in Ref. 4 is that in the quaternion case, the unitary matrix factors must always be ordered to the right of ket state vectors, whereas in the complex case the ordering is irrelevant, and in fact in Ref. 4 the matrix factors are ordered to the left. The results of Ref. 4 can be obtained by the complex specialization of the results obtained in this paper. However, we have introduced here a new technique of using parallel transported states $|\hat{\psi}_a\rangle$ to cleanly separate the non-Abelian geometric phase and the dynamical phase, which in general (even in the complex non-Abelian case) do not commute with each other.

5. Summary and Discussion

To summarize, we have shown that both the complex Abelian and non-Abelian nonadiabatic geometric phases can be generalized to quaternonic Hilbert space. These results are both of theoretical interest, and of experimental relevance for possible tests for complex versus quaternionic quantum mechanics. Long ago, Peres [8] proposed testing for quaternionic quantum mechanical effects by looking for noncommutativity of scattering phase shifts. However, the result of Ref. 6 that the S-matrix in quaternionic quantum mechanics is always complex valued (for nonzero energy states) implies that there are no quaternionic scattering phase shifts, and the Peres test necessarily gives a null result. An alternative but related method is to look for interference effects in cyclic evolutions that could show the presence of quaternionic effects. The fact [6] that the adiabatic geometric phase is always complex (for nonzero energy states) is a counterpart of the complexity of the S-matrix, and implies that a null result will always be obtained for cyclic interference experiments involving adiabatic state evolutions. However, the results obtained here show that for cyclic evolutions that are nonadiabatic, one could in principle devise interference experiments to place meaningful bounds on postulated quaternionic components of the wave function.

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